

Deviations from Universality and the Contact in finite range interacting ultracold Fermi systems

Santiago F. Caballero-Benítez, Rosario Paredes and Víctor Romero-Rochín

Instituto de Física, Universidad Nacional Autónoma de México,

Apdo. Postal 20-364, México D. F. 01000, México.

(Dated: April 26, 2012)

Using the Bardeen-Cooper-Schrieffer (BCS) ansatz, we investigate the deviations in the behavior of ground state thermodynamic properties of an interacting homogenous Fermi gas from the zero range interaction approximation. The considered finite range interatomic potential allows us to vary the strength of the interaction to study the whole crossover from the BCS limit to the Bose-Einstein condensation (BEC) limit with no approximations. In particular, we concentrate in analyzing the thermodynamic *Contact* variable across the weak and strong coupling limits. Our analysis validates the correctness of the zero range approximation (contact approximation) in the strongly interacting regime. We predict quantum phase transition-like behaviour for long range interatomic potentials. These findings follow from an energy dependent gap due to the finite range of the interatomic potential.

The experiments performed on dilute ultracold two-component Fermi gases represent perhaps the cleanest scenario that allows to access the crossover from Bardeen-Cooper-Schrieffer (BCS) superfluidity of Cooper pairs to Bose-Einstein condensation (BEC) of tightly bound fermion pairs [1–6]. These systems can be appropriately modelled by a Hamiltonian describing interacting fermions in a homogeneous environment. Inhomogeneities created by a confining potential may be included via the local density approximation (LDA) [7]. Although the study of the crossover has been extensively addressed in the literature at zero [8–25] and non-zero temperatures [26, 27], still, important issues remain to be discussed. One of them refers to the recently identified contact variable [28], which besides from being amenable to direct measurement, yields information on a host of different properties, among them, density-density correlations [29], the number of pairs in the closed channel of a Feshbach resonance [30, 31], and on the forms of thermodynamic variables at unitarity [28]. Additionally, as we argue below, the calculation of this quantity is very sensitive to different approximations and schemes. In this Letter, we readdress the crossover within the BCS mean-field theory (MF) but *without* making the usual contact approximation in the interatomic interaction potential, $U(r) \approx \delta(r) \frac{4\pi\hbar^2 a}{m}$ where a is the s-wave scattering length. Namely, we calculate the thermodynamics at zero temperature for a realistic finite range potential. Although there have been previous analysis with finite-range interatomic potentials [32, 33], the issues addressed here have not been discussed.

The system is a balanced mixture of two monoatomic fermionic species with the same atomic mass m , and whose interatomic potentials is $U(|r - r'|)$. The Hamiltonian in momentum space is given by

$$H = \sum_k \epsilon_k (\hat{a}_k^\dagger \hat{a}_k + \hat{b}_k^\dagger \hat{b}_k) + \frac{1}{V} \sum_{kk'q} \tilde{U}_q \hat{a}_{k+q}^\dagger \hat{b}_{k'-q}^\dagger \hat{b}_{k'} \hat{a}_k$$

$$+ \frac{1}{2V} \sum_{kk'q} \tilde{U}_q [\hat{a}_{k+q}^\dagger \hat{a}_{k'-q}^\dagger \hat{a}_{k'} \hat{a}_k + \hat{b}_{k+q}^\dagger \hat{b}_{k'-q}^\dagger \hat{b}_{k'} \hat{b}_k] \quad (1)$$

where V is the volume that confines the sample, $\epsilon_k = \hbar^2 k^2 / 2m$ is the energy of a particle with momentum $\pm \hbar k$. \hat{a}_k and \hat{b}_k are the annihilation operators of the two different species and obey anticommutation rules. \tilde{U}_q is the Fourier transform of the interatomic potential $U(r)$. Here, for simplicity we have assumed that the interatomic potential is the same for any pair of fermions.

The BCS ansatz [34–36] for the ground state of the gas assumes that this state is a superposition of all possible Cooper pairs in the fluid, $|\Psi_{\text{BCS}}\rangle = \prod_k (u_k + v_k \hat{a}_k^\dagger \hat{b}_{-k}^\dagger) |0\rangle$ being u_k and v_k variational parameters with the property $u_k^2 + v_k^2 = 1$ ensuring the normalization of the state. A straightforward evaluation in the grand canonical ensemble of the expectation value of the grand potential $\Omega = \langle \Psi_{\text{BCS}} | H - \mu [\sum_k (\hat{a}_k^\dagger \hat{a}_k + \hat{b}_k^\dagger \hat{b}_k)] | \Psi_{\text{BCS}} \rangle$, where the common chemical potential μ for A and B species ensures that the mixture is balanced, yields

$$\Omega = 2 \sum_k (\epsilon_k - \mu + \epsilon_k^{HF}) v_k^2 + \frac{1}{V} \sum_{kk'} \tilde{U}_{k-k'} F_k F_{k'}, \quad (2)$$

where $F_k = u_k v_k$. The term ϵ_k^{HF} stands for the Hartree and Fock energy contributions, given by,

$$\epsilon_k^{HF} = \frac{\tilde{U}_0}{V} \sum_{k'} v_{k'}^2 - \frac{1}{2V} \sum_{k'} \tilde{U}_{k-k'} v_{k'}^2. \quad (3)$$

A straightforward variational scheme requiring that $\partial\Omega/\partial v_k = 0$ for all k , yields the well known equation for the gap,

$$\Delta_k = -\frac{1}{V} \sum_{k'} \tilde{U}_{k-k'} \frac{\Delta_{k'}}{2E_{k'}}, \quad (4)$$

where the quasiparticle excitation energy is $E_k = [(\epsilon_k - \mu + \epsilon_k^{HF})^2 + \Delta_k^2]^{1/2}$. One supplements the above equations with the total number of particles $N = 2 \sum_k v_k^2$.

The above equations are valid for any short range interatomic potential. The contact approximation [36] is implemented by setting all the momenta dependence as $\tilde{U}_q \approx \tilde{U}_0 \equiv \frac{4\pi\hbar^2 a}{m}$, and as it is well known, such a procedure inevitably leads to convergence difficulties at large values of the momentum q , with the necessity of either, schemes of renormalization nature or introducing physically justified cut-off parameters [36, 37]. This approximation disregards the significant role of the range σ of the interatomic potential in determining the physics of the problem. In order to avoid this approximation we use a physically acceptable interatomic potential, an exponential-type of potential,

$$U(r) = -V_0 e^{-r/\sigma} \quad (5)$$

where V_0 is the depth of the potential, and whose Fourier transform is

$$\tilde{U}_k = -\frac{8\pi V_0 \sigma^3}{(1 + k^2 \sigma^2)^2}. \quad (6)$$

This potential has essentially two main virtues. First, as a realistic potential it depends on at least two parameters, V_0 and σ . Second, but more important for our purposes, as derived by Rarita [38], the two-body scattering length is exactly known,

$$a = -2\sigma \left[\frac{\pi N_0(x)}{2 J_0(x)} - \ln \left(\frac{x}{\sqrt{2}} \right) - \gamma \right], \quad (7)$$

where $x = \sigma\sqrt{2V_0 m}/\hbar$, $J_0(x)$ and $N_0(x)$ are zero order Bessel functions of first and second kind respectively with γ , the Euler-Mascheroni constant. Therefore, for fixed range σ , the Grand Potential Ω depends on the scattering length via V_0 . As V_0 varies, a passes through an infinite series of scattering resonances where a diverges changing abruptly its sign; the resonances occur as actual bound states emerge [38]. As it has also been widely discussed, those potential resonances are good approximations to experiments since essentially all crossover experiments are in the so-called broad Feshbach resonance limit where the width of the resonance is much larger than the Fermi energy [29, 33, 39]. In this study we consider the BCS-BEC crossover through the first resonance.

To analyze the thermodynamics in the whole BCS-BEC crossover, namely, as the *inverse* scattering length varies from $-\infty$ to ∞ , we numerically solve [40] the set of equations (4)-(7) without any further assumption or approximation. Although not an independent thermodynamic variable, we also discuss the behavior of the energy dependent gap Δ_k . Unlike the standard BCS-BEC crossover mean-field theory by Leggett, the use of a finite range potential causes this energy dependence. We determine the chemical potential μ , the pressure $p = -\Omega/V$ and the contact variable \mathcal{C} given by [28, 30, 41]

$$\mathcal{C} = - \left(\frac{\partial \Omega}{\partial \eta} \right)_{\mu, V, T}. \quad (8)$$

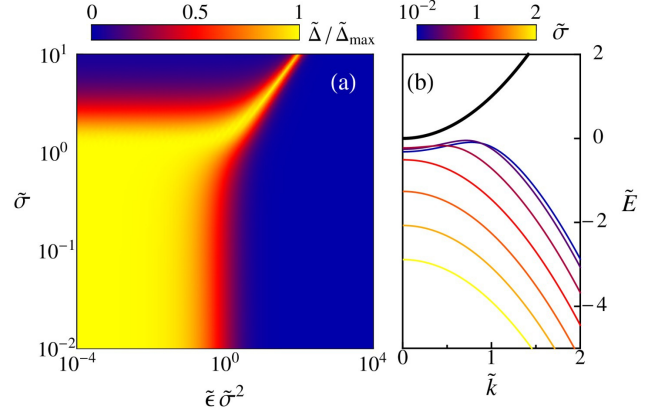


FIG. 1. (color online) (a) Dimensionless gap $\tilde{\Delta}/\tilde{\Delta}_{\max}$ as a function of interatomic interaction range $\tilde{\sigma}$ and as a function of the scaled energy $\tilde{\epsilon}\tilde{\sigma}^2$, with $\tilde{\epsilon} = \epsilon_k/\epsilon_F$. (b) Quasiparticle excitation energy, $\tilde{E} = \tilde{\mu} - \tilde{E}_{\tilde{k}}$, for different values of the potential range $\tilde{\sigma}$. The thick line corresponds to \tilde{k}^2 . These calculations correspond to $\tilde{\eta} = 0$.

All variables can be adimensionalized in terms of the Fermi energy and momentum, $\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$ and $k_F = (3\pi^2 \frac{N}{V})^{1/3}$. The corresponding dimensionless variables will be denoted with a tilde. In this way, the dependence on density N/V is implicit and we are left with a dependence on the inverse of the scattering length $\eta = 1/a$ and on the range of the potential σ only.

To begin our discussion, we show in Fig.1 (a) the normalised gap $\tilde{\Delta}(\tilde{\epsilon}, \tilde{\sigma})/\tilde{\Delta}_{\max}(\tilde{\sigma})$, as a function of $\tilde{\epsilon} = \epsilon_k/\epsilon_F$ and $\tilde{\sigma} = \sigma/k_F$, where $\tilde{\Delta}_{\max} = \max[\tilde{\Delta}(\tilde{\epsilon}, \tilde{\sigma})]$. Although these calculations were performed for the strongly interacting regime ($\tilde{\eta} = 0$), the results are completely general in comparison with other values of the scattering length. We find that as long as $\tilde{\sigma} \lesssim 1$, the gap is a constant $\tilde{\Delta} \approx \tilde{\Delta}_{\max}$ for $\tilde{\epsilon}\tilde{\sigma}^2 \lesssim 1$, then abruptly drops to zero. As $\tilde{\sigma} \rightarrow 0$, we recover a constant gap for all $\tilde{\epsilon}$. For moderate and large values of $\tilde{\sigma}$, the gap shows a peak. As we see below, this novel dependence of the gap for large values of \tilde{k} dramatically changes the behavior of the thermodynamic properties. To complement the facts provided by the dependence of the ground state properties on the non-zero range potential, in Fig.1 (b) we plot the behavior of the quasiparticle excitation energy \tilde{E}_k for several values of $\tilde{\sigma}$. These results are in good agreement with those obtained for finite temperatures [42].

We now address the main point of this letter. This is the behavior of the contact variable \mathcal{C} , eq. (8), for the whole crossover at $T = 0$. In addition to its physical relevance, we discuss the contact variable because it has been noted recently [30] that \mathcal{C} is very sensitive to the contact approximation in the BCS mean-field approach. Fig. 2 (a) shows $\tilde{\mathcal{C}} = \mathcal{C}k_F/(N\epsilon_F)$ as a function of $\tilde{\eta} = 1/(k_F a)$ for different values of the dimensionless range $\tilde{\sigma}$. First, we highlight the dashed black line that corresponds to

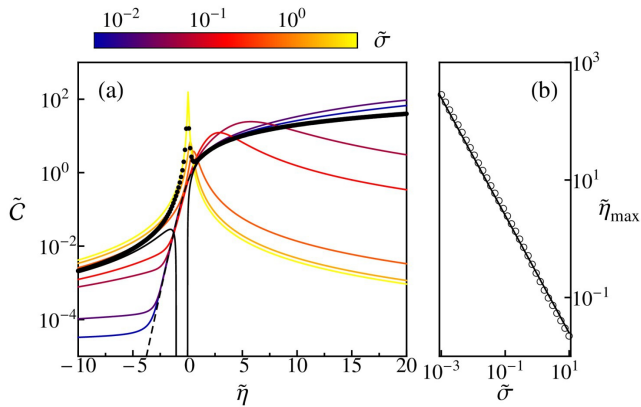


FIG. 2. (color online) (a) Dimensionless contact variable $\tilde{C} = \mathcal{C}k_F/(N\epsilon_F)$ as a function of inverse scattering length $\tilde{\eta} = 1/(k_F a)$. The color curves are the results of the full BCS equations for finite values of $\tilde{\sigma}$, coded in the colored bar above. The dotted line is the BCS solution in the contact approximation neglecting the HF terms. The continuous black lines are HYL limit. (b) The value of $\tilde{\eta}_{\max}$ where the contact takes its maximum value. We note that it obeys a very simple scaling $\tilde{\eta}_{\max} \approx 1/(4\tilde{\sigma})$.

the solution of the BCS equations in the contact approximation but completely *neglecting* the Hartree-Fock (HF) terms, see eq. (2). This approximation has been deemed as inappropriate [30] to describe the system since in the deep BCS regime, $\tilde{\eta} \rightarrow -\infty$, it predicts an exponential decay, as can be seen in Fig. 2 (a) [dashes].

The correct behavior of \tilde{C} is believed to be given by the weakly-interacting approximations of a Fermi liquid in the BCS side and the diatomic version of a Bose gas with repulsive interactions in the BEC side. Both are the celebrated expressions of Huang-Yang-Lee (HYL) [43]. In the very deep BCS and BEC regimes, those are simply HF corrections. In the BCS side one finds that the leading term is $\tilde{C} \approx 2/(3\pi\tilde{\eta}^2)$ while in the BEC side $\tilde{C} \approx 2\tilde{\eta}$. These are shown with solid black lines in Fig. 2 (a). As expected, the crossover cannot be described within such an approximation. In addition to these lines, with black dots, we also plot the mean-field BCS theory, in the contact approximation, *with* the HF terms. We see that as $\tilde{\eta} \rightarrow \pm\infty$, this solution approaches HYL result but, in the strongly interacting limit diverges. The latter behavior does appear to invalidate the use of mean-field theory. However, the divergence is due to the contact approximation and not to the mean-field approach itself, as we discuss now. In color lines we show the finite range calculations. In general, we find that as $\tilde{\sigma}$ is very small, the contact \tilde{C} vanishes algebraically as $\tilde{\eta}^{-2}$, in partial agreement with HYL. The actual HYL behavior is followed for $\tilde{\sigma} \sim 1$, while for $\tilde{\sigma} \ll 1$ this behavior appears for much larger $-\tilde{\eta}$. We deduce from the finite range calculations that in the limit $\tilde{\sigma} \rightarrow 0$ the HYL contributions become less important and the BCS theory with contact

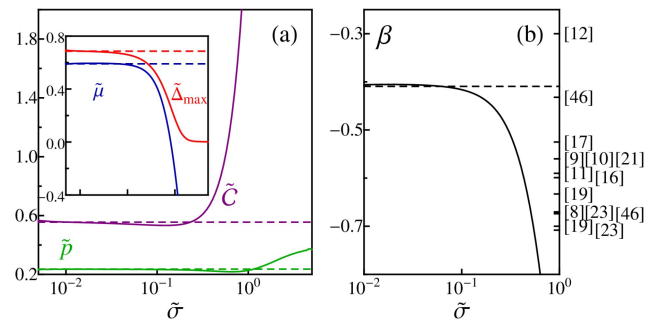


FIG. 3. (color online) Thermodynamics at unitarity $\tilde{\eta} = 0$. (a) The chemical potential $\tilde{\mu}$, the maximum value of the gap $\tilde{\Delta}_{\max}$, the pressure \tilde{p} and the contact variable \tilde{C} , as functions of the interaction range $\tilde{\sigma}$. (b) Bertsch parameter β as a function of $\tilde{\sigma}$. The numbers on the right correspond to references of different calculations. Dashed lines correspond to the predicted values at unitarity of the BCS theory in the contact approximation *without* the Hartree-Fock terms. All quantities are dimensionless.

approximation, but *without* HF terms is the correct result. In the BEC side a novel behavior emerges due to the finite character of $\tilde{\sigma}$. The contact variable \tilde{C} peaks at a value that depends on $\tilde{\sigma}$ and then decays to zero again as $\tilde{\eta}$ increases. The value of $\tilde{\eta}_{\max}$ at the peak scales simply as $\tilde{\sigma}^{-1}$, see Fig. 2 (b). We further note that as $\tilde{\sigma}$ keeps increasing, the location of the peak not only tends to $\tilde{\eta} = 0$, i.e. to unitarity, but the value of \tilde{C} becomes sharply peaked, suggesting that the crossover at unitarity becomes a true quantum phase transition. Although the transition may appear unrealistic since one needs an infinite interatomic range, we would like to recall that the present theory is a mean-field one. Such a transition is reminiscent of the Kac limit [44] of the van der Waals fluid. The latter is the epitome of the equation of state of a real fluid, showing both first and second order phase transitions, yet it does not represent any real fluid. It remains to experimentally verify whether the present Kac limit is a precursor of a true phase transition for real atoms with finite range interactions.

In the unitary limit ($|a| \rightarrow \infty$) the interactions are strong and in the zero range limit the system possesses universal properties [45]. However, in the contact approximation the HF terms in the Hamiltonian [last line (1)] become divergent at unitarity. We find that by using a finite range interatomic potential the terms are finite and are clearly not proportional to the scattering length. Moreover, the contact approximation can only be used in the weakly interacting regime. Since in our treatment, we never use the contact approximation, we never face any divergence. Thus, we find that the crossover in general is smooth as one would expect, except when $\tilde{\sigma} \gg 0$ where the system approaches the Kac limit [44]. First, we note that, as $\tilde{\sigma} \lesssim 1$, the exact calculation approaches that of the usual BCS mean-field calculation with the

contact approximation, but *without* including the divergent HF terms, dotted lines in Fig. 3. We have that for small interatomic range, all thermodynamic quantities approach the MF universality class [45]. For larger values of $\tilde{\sigma}$ evident deviations appear. In Fig. 3 (b) we show Bertsch parameter $\beta = E_{\text{Int}}/E_0 - 1$ [46] (E_{Int} and E_0 are the energies of the interacting system and non-interacting system respectively) for the present calculation together with a collection of corresponding values

for different type of models and calculations [8–12, 15–17, 19, 21, 23, 46]. We clearly see that all those values are within $\tilde{\sigma} \lesssim 1$ of the exact calculation using the BCS ansatz. As one would expect, as the interaction range increases at unitarity the system starts to deviate strongly from the ideal Fermi gas ($\beta = 0$) and the result of the contact approximation ($\beta = -0.41$). Full elucidation of this important point is beyond the scope of this article.

This work was partially supported by grant IN108812-2 DGAPA (UNAM).

-
- [1] M. Greiner M, C.A. Regal and D.S. Jin, Nature **426**, 537 (2003).
 - [2] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, S. Riedl, C. Chin, J.H. Denschlag and R. Grimm, Science **302**, 5653 (2003).
 - [3] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, S. Gupta, Z. Hadzibabic, and W. Ketterle, Phys. Rev. Lett. **91**, 250401(2003).
 - [4] T. Bourdel, L. Khaykovich, J. Cubizolles, J. Zhang, F. Chevy, M. Teichmann, L. Tarruell, S. J. J. M. F. Kokkelmans, and C. Salomon, Phys. Rev. Lett. **93**, 050401 (2004).
 - [5] J. Kinast, S. L. Hemmer, M. E. Gehm, A. Turlapov, and J. E. Thomas, Phys. Rev. Lett. **92**, 150402 (2004).
 - [6] G. B. Partridge, K. E. Strecker, R. I. Kamar, M. W. Jack, and R. G. Hulet, Phys. Rev. Lett. **95**, 020404 (2005).
 - [7] S. Giorgini, L. P. Pitaevskii and S. Stringari, Rev. Mod. Phys. **80** 1215 (2008).
 - [8] H. Heiselberg, Phys. Rev. A **63**, 043606 (2001).
 - [9] J. Carlson, S.-Y. Chang, V. R. Pandharipande, and K. E. Schmidt, Phys. Rev. Lett. **91** 050401(2003).
 - [10] S. Y. Chang, V. R. Pandharipande, J. Carlson, and K. E. Schmidt, Phys. Rev. A **70** 043602 (2004).
 - [11] J. Carlson and S. Reddy, Phys. Rev. Lett. **95**, 060401 (2005).
 - [12] G. M. Bruun, Phys. Rev. A **70**, 053602 (2004).
 - [13] A. Perali, P. Pieri, and G. C. Strinati, Phys. Rev. Lett. **93** 100404 (2004).
 - [14] P. Pieri, L. Pisani, and G. C. Strinati, Phys. Rev. B **70**, 094508 (2004).
 - [15] G. E. Astrakharchik, J. Boronat, J. Casulleras, and S. Giorgini, Phys. Rev. Lett. **93** 200404 (2004).
 - [16] H. Hu, X.-J. Liu and P. D. Drummond, Europhys. Lett. **74**, 574 (2006).
 - [17] Y. Nishida and D. T. Son, Phys. Rev. Lett. **97**, 050403 (2006).
 - [18] J. von Stecher, Chris H. Greene, and D. Blume, Phys. Rev. A **77** 043619 (2008).
 - [19] P. Arnold, J. E. Drut and D. T. Son. Phys. Rev. A **75**, 043605 (2007).
 - [20] R. Jauregui, R. Paredes, and G Toledo Sanchez, Phys. Rev. A **76** 011604 (2007).; R. Jauregui, R. Paredes, L. Rosales-Zarate and G. Toledo Sanchez, J. Phys. B: At Mol. Opt. Phys. **43** 065301 (2010).
 - [21] S. Y. Chang, Phys. Rev. A **77**, 051602(R) (2008).
 - [22] A. Gezerlis and J. Carlson, Phys. Rev. C **77**, 032801(R) (2008).
 - [23] D. Lee, Phys. Rev. C **78**, 024001 (2008).
 - [24] S. K. Adhikari, Phys. Rev. A **79** 023611 (2009).
 - [25] X. Leyronas and R. Combescot, Phys. Rev. Lett. **99**, 170402 (2007).
 - [26] P. Nozières, and S. Schmitt-Rink, J. Low Temp. Phys. **59**, (1985).
 - [27] C.A.R. Sá de Melo, M. Randeria, and J. R. Engelbrecht, Phys. Rev. Lett. **71**, 3202 (1993).
 - [28] S. Tan, Ann. Phys. (NY) **323** 2971 (2008), S. Tan, Ann. Phys. (NY) **323** 2952 (2008), S. Tan, Ann. Phys. (NY) **323** 2987 (2008).
 - [29] W. Zwerger, Ed. *The BCS-BEC Crossover and the Unitary Fermi Gas*, Springer-Verlag Berlin Heidelberg (2012).
 - [30] F. Werner, L. Tarruell and Y. Castin, Eur. Phys. J. B **68** 401 (2009).
 - [31] S. Zhang and A.J. Leggett, Phys. Rev. A **79**, 023601 (2009).
 - [32] M.M. Parish, B. Mihaila, E.M. Timmermans, K.B. Blagoev, and P.B. Littlewood, Phys. Rev. B **71**, 064513 (2005).
 - [33] C. Chin, R. Grimm, P.S. Julienne and E. Tiesinga, Rev. Mod. Phys. **82**, 1225 (2010).
 - [34] J. Bardeen, L.N. Cooper and J.R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
 - [35] D.M. Eagles, Phys. Rev. **186** 456 (1969).
 - [36] A.J. Leggett in *Modern Trends in the Theory of Condensed Matter* (Berlin, Springer) **115**13 (1980).
 - [37] L.P. Gorkov, Sov. Phys. JETP **7**, 505 (1958).; L.P. Gorkov and T.K. Melik-Barkhudarov, Sov. Phys. JETP **13**, 1018 (1961).
 - [38] W. Rarita and R.D. Present, Phys. Rev. **51** 788 (1937).
 - [39] T. Kölher, K. Goral and P.S. Julienne, Rev. Mod. Phys. **78**, 1311 (2006).
 - [40] We use a series of relaxation routines. W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C. The Art of Scientific Computing*, 2nd ed. (Cambridge University Press, New York, 1992). The numerical code for the solution of eqs.(4)-(7) is available under request.
 - [41] V. Romero-Rochín, J. Phys. B: At. Mol. Opt. Phys. **44** 095302 (2011).
 - [42] J. P. Gaebler1, J. T. Stewart, T. E. Drake, D. S. Jin, A. Perali, P. Pieri and G. C. Strinati, Nature Phys. **6**, 569 (2010).
 - [43] K. Huang, C.N. Yang, Phys. Rev. **105**, 767 (1957); T.D. Lee and C.N. Yang, Phys. Rev. **105**, 1119 (1957).
 - [44] M. Kac, G. E. Uhlenbeck, and P. C. Hemmer, J. Math. Phys. **4**, 216 (1963), M. Kac, G. E. Uhlenbeck, and P. C. Hemmer, J. Math. Phys. **4**, 229 (1963), M. Kac, G. E. Uhlenbeck, and P. C. Hemmer, J. Math. Phys. **5**, 60

- (1964);
- [45] T-L Ho, Phys. Rev. Lett. **92**, 090402 (2004).
- [46] G.F. Bertsch, in *Proceedings of the Tenth International Conference on Recent Progress in Many-Body Theories*, edited by R.F. Bishop et al. (World Scientific, Singapore 2000).; G. A. Baker Jr., Phys. Rev. C **60**, 054311 (1999).